International Journal of
QUANTUM CHEMISTRY

Contents for Volume 47, 1993, Nos. 1–6 and 48, 1993, Nos. 1–6

Issue No. 1, 1993

Editorial
P.-O. Löwdin 1

Diagrammatic Analysis and Application of the Coupled Cluster Response Approach to Ground-State Expectation Values
M. Nooijen and J. G. Snijders 3

The Tautomers of Uracil: A Local Correlation Treatment
J. W. Boughton and P. Pulay 49

Electronic Structure of DNA Dimer-Units, d(AA) · d(TT), $d(TA)_2$, $d(AT)_2$, in A and B Conformations by DV-Xα Cluster Calculations
T. Shinoda, N. Shima, and M. Tsukada 59

Gaussian Expansions from STOs by the Distance Between Subspaces
J. M. Garcia de la Vega and B. Miguel 85

Book Review

Density-Functional Theory of Atoms and Molecules. By R. G. Parr and W. Yang
J.-L. Calais 101

Guidelines for Preparing an Electronic Manuscript I

Issue No. 2, 1993

Perturbation–Variational Methods Revisited
M. R. Chacon and M. C. Zerner 103

A Study of Excited States in *trans*-Polyacetylene in the Hartree–Fock, Tamm–Dancoff, and Random-Phase Approximation
M. G. Vracko and M. Zaider 119

Dipole, Quadrupole, Octupole, and Dipole–Dipole–Quadrupole Polarizabilities and Second Hyperpolarizabilities at Real and Imaginary Frequencies for Helium in the 2^3S State. Dispersion-Energy Coefficients for Interactions Between He(2^3S) and H(1^2S), He(1^1S), He(2^3S), or $H_2(X^1\Sigma_g^+)$
D. M. Bishop and J. Pipin 129

A Numerical Integration Scheme for the Evaluation of Correlation Energy Functionals
A. Fortunelli and O. Salvetti 135

Decomposition and Interpretation of the SCF Interaction and Deformation Energies by the Modified Pauli Blockade Method
K. Pecul 145

A Mutually Consistent Procedure for Excitation Energies and Transition Densities Based on the Extended Brillouin's Theorem
Y. Yu. Dmitriev, A. O. Mitrushenkov, M. P. Fülscher, and B. O. Roos .. 155

Erratum

Redshifts and Blueshifts of OH Vibrations
K. Hermansson 175

Guidelines for Preparing an Electronic Manuscript I

Issue No. 3, 1993

Effect of Positive Background on the Ground-State Energy of a Wigner Lattice
I. Sebasdiyar, K. Iyakutti, and M. Mahendran 177

A Scheme for Representation Matrices of a Permutation Group Using Spin-Paired Functions
C. Kadolkar, C. R. Sarma, and D. K. Ghosh 185

Examination of the Hund Rule in Closed-Shell Systems: Investigation of Spin Correlation Effects
R. Martín Parrondo, P. Karafiloglou, and E. Sánchez Marcos 191

Decay Dynamics of a Metastable State in a Time-Varying Electric Field: A Three-Level Prototypical System
S. Adhikari, S. P. Bhattacharyya, and D. M. Bhattacharyya 213

Computation of Many-Center Exchange Integrals over Slater Orbitals up to 4*d* by Means of Optimized Gaussian Expansions
R. Montagnani and O. Salvetti 225

Helical Region of the Potential Energy Surface of α-Aminoisobutyric Acid: A Theoretical Study
C. Alemán and J.J. Perez 231

Book Review

Quanta a Handbook of Concepts, Second Edition. By P.W. Atkins
A. Strich 239

Guidelines for Preparing an Electronic Manuscript I

Issue No. 4, 1993

Products of Class-Sums of the Symmetric Group: Generalizing the Recurrence Relations
J. Katriel 243

MAPLE Symbolic Computation of the Long-Range Many-Body Intermolecular Potentials: Three-Body Induction Forces Between Two Atoms and a Linear Molecule
P. Piecuch 261

Intrinsic Reaction Coordinate of Perturbed Potential Energy Surfaces: Construction of Perturbed Energy Profiles
J. Mestres and M. Duran 307

A Simple Proof for the Formula to Get Symmetrized Powers of Group Representations
J. Planelles and C.M. Zicovich-Wilson 319

Diskette Submission Instructions I

Issue No. 5, 1993

Electronic-Phase of the Hartree–Fock Solution of the Infinite One-Dimensional System: Structural Change in an Arbitrarily Doped Polyacetylene Chain
K. Tanaka, A. Takata, M. Okada, and T. Yamabe 325

Ab Initio Potential Energy Function for the Dynamics of the Fluoronium Ion
F. A. Gianturco, E. Buonomo, E. Semprini, F. Stefani, and A. Palma 335

Selective Dynamic Energy Transfers in Proton Collisions with Hydrogen Fluoride
F. A. Gianturco, E. Buonomo, and S. Serna 375

Binding Regions in Polyatomic Molecules
X. Wang and Z. Peng 393

Diskette Submission Instructions I

Issue No. 6, 1993

Accurate Computation of Eigenfunctions for Schrödinger Operators in One Dimension
M. A. Núñez and G. Izquierdo B. 405

Relativistic Theory for Indirect Nuclear Spin–Spin Couplings within the Polarization Propagator Approach
G. A. Aucar and J. Oddershede 425

Temperature Dependence of Hydrogen Transfer Reactions Via Tunneling at Low Temperatures
A. K. Chandra and V. S. Rao 437

Electronic Structures around the Local Defects in All-*trans*-Polyacetylene: An Analysis by the Cluster-Series Model
K. Maekawa and A. Imamura 449

Rayleigh–Schrödinger Perturbation Theory for Nonlinear Schrödinger Equations with Linear Perturbation
J. G. Ángyán 469

Diskette Submission Instructions I

Vol. 48, Issue No. 1, 1993

Electron Correlation Effects in the Rydberg-like 3^3D and 3^1D States of Helium-like Ions
N. M. Cann, R. J. Boyd, and A. J. Thakkar 1

Coupled Cluster Green's Function Method: Working Equations and Applications
M. Nooijen and J. G. Snijders 15

Electronic Structures of High-T_c Superconductors $LnBa_2Cu_3O_7$ (Ln = Pr, Nd, Gd, Dy)
M. Li 49

Multiple Solutions of the Valence-Universal Coupled-Cluster Equations for Be, B^+, and C^{2+}
K. Jankowski and P. Malinowski 59

Diskette Submission Instructions I

Issue No. 2, 1993

Molecular Surface Electrostatic Potentials and Local Ionization Energies of Group V–VII Hydrides and Their Anions: Relationships for Aqueous and Gas-Phase Acidities
T. Brinck, J. S. Murray, and P. Politzer 73

Early Stages of LiX, BeH_2X, and BH_3X Pyrolysis (X Stands for NH_3 or OH_2): A Theoretical Study of Weak Dative Complex Stability
M. Sana and G. Leroy 89

On the Car–Parrinello Computational Scheme: Rigorous Treatment
E. S. Kryachko 109

Eigenvalues of Single-Cycle Class-Sums in the Symmetric Group. II
J. Katriel and R. Pauncz 125

Stable Electronic Energy Levels in the Presence of Off-Diagonal Disorder
I. László 135

Book Review

Quantum Field Theory: A Modern Introduction. By Michio Kaku
J. R. Klauder 147

Diskette Submission Instructions I

Issue No. 3, 1993

Nonlinear Roothaan's Equations
J. Marañón 151

Explicitly Connected Expansion for the Average Value of an Observable in the Coupled-Cluster Theory
B. Jeziorski and R. Moszynski 161

A First-Principles Approach to High-T_c Superconductivity. I. A Consistent One-Electron Theory of the N-Electron Problem
L. Fritsche 185

A First-Principles Approach to High-T_c Superconductivity. II. The Superconducting Ground State
L. Fritsche 201

Finding Transition States When Second-Order Jahn–Teller Instability Occurs
J. Simons 211

Diskette Submission Instructions I

Issue No. 4, 1993

Ground and First Excited States of Fractionally Charged Sodium Atoms
A. C. Pavão, J. S. Craw, and M. A. C. Nascimento 219

Some Remarks on the Resemblance Theorems Associated with Various Orthonormalization Procedures
P.-O. Löwdin 225

Electric-Field Mapping of Some Anions and Cations of Adenine and Guanine
C. G. Mohan, A. Kumar, and P. C. Mishra 233

Multiplication Theorems for Orthogonal Polynomials
H. Kleindienst and A. Lüchow 239

Perturbation Theory to Determine the Stable Isomer of Triatomic Linear Molecules
M.-D. Su 249

Recurrence Relations for the Evaluation of Electron Repulsion Integrals over Spherical Gaussian Functions
A. Fortunelli and O. Salvetti 257

The Low-Lying Excitation Energies of Polyenes Investigated with a Chain-Length-Dependent Screened Potential
R. E. Siregar and M. O. Tjia 267

Diskette Submission Instructions I

Issue No. 5, 1993

Geometrical, Spectroscopic, and Magnetic Properties of an Oxygen Atom Adsorbed on the Ni(100) Surface
A. Goursot, F. Mele, N. Russo, D. R. Salahub, and M. Toscano 277

Topological Analysis of the Charge Density of Solids: *bcc* Sodium and Lithium
C. Mei, K. E. Edgecombe, V. H. Smith, Jr., and A. Heilingbrunner ... 287

Multipole Moment Analysis for Hydrides, Fluorides, and Lithium Compounds of First- and Second-Row Elements
A. M. Köster and K. Jug 295

Second-Order Jahn–Teller Instability and the Activation Energy for $Al^+(^1S) + H_2 \rightarrow AlH^+(^2\Sigma^+) + H$
J. Rusho, J. Nichols, and J. Simons 309

Fluorination Effect on the Structural Properties in Benzocyclobutenes and Benzocyclobutadienes
W. Koch, M. Eckert-Maksić, and Z. B. Maksić 319

Electronic Structure and Hyperpolarizability of Some Conjugated Molecules in Excited States
I. Kanev 333

Diskette Submission Instructions I

Issue No. 6, 1993

Semiempirical Evaluation for Proton Affinities of Phosphorus Compounds
A. B. Pierini and J. S. Duca, Jr. 343

Valence Electronic States of NH^{2+} and PH^{2+} Dications
J. K. Park and H. Sun 355

Molecular Calculations Using Space-Restricted Basis Functions
P. L. Goodfriend and S. I. Tsonchev 367

Some Comments on the Counterpoise Correction for the Basis Set Superposition Error at the Correlated Level
D. B. Cook, J. A. Sordo and T. L. Sordo 375

Announcement 385

Volume Title Page 387

Subject Index to Volumes 47 and 48 389

Volume Contents 393

Author Index to Volumes 47 and 48 401

Diskette Submission Instructions I